

# Time-dependent transport via a quantum shuttle

M. Tahir\* and A. MacKinnon

*Department of Physics, The Blackett Laboratory, Imperial College London,  
South Kensington Campus, London SW7 2AZ, United Kingdom*

We present a theoretical study of time-dependent transport via a quantum shuttle within the non-equilibrium Green's function technique. An arbitrary voltage is applied to the tunnel junction and electrons in the leads are considered to be at zero temperature. The transient and the steady state behavior of the system is considered here in order to explore the quantum dynamics of the shuttle device as a function of time and applied bias. The properties of the phonon distribution of the oscillating dot coupled to the electrons are investigated using a non-perturbative approach. We derive a relation for the oscillator momentum charge density correlation function which is an interesting physical example for the visualization of shuttling phenomenon. We consider the crossover between the tunneling and shuttling regimes for different values of the key parameters as a function of applied bias and time. We also consider the energy transferred from the electrons to the oscillating dot as a function of time. This will provide useful insight for the design of experiments aimed at studying the quantum behavior of a shuttling device.

## I. INTRODUCTION

In recent years, there has been a great interest in the study of transport phenomena through nanoelectromechanical systems (NEMS)[1–4] both at an applied and at fundamental level. This attention has been focused due to the fact that novel transport regimes arise due to strong interplay between electrical and mechanical degrees of freedom, which promise both the concept and realization of these systems as a new generation of quantum electromechanical devices. A large number of new experimental techniques have been developed to fabricate and perform experiments with NEMS in the quantum regime; Examples of high-frequency mechanical nano-structures that have been produced are nano-scale resonators[5, 6], semiconductor quantum dots and single molecules[7–11], cantilevers[12, 13], vibrating crystal beams[5] and more recently graphene sheets[14] and carbon nanotubes[15, 16]. Anticipated quantum effects[5, 6, 12, 13, 17] include observation of single phonons as well as ground state effects such as zero point displacement, ultra small mass sensing, measurement of extremely weak forces and suppression of scattering in coupled electromechanical systems. The strong interplay between a phonon mode and electrons is crucial for observing the quantum effects in the transport of charge through electromechanical systems.

A special kind of electromechanical system where the interplay between the electrical and mechanical degrees of freedom drastically changes the transport properties is a shuttling device[7, 18, 19]. The characteristic component that gives the name to these devices is an oscillating quantum dot of nanometer size that transfers electrons one-by-one between a source and a drain lead. A shuttling device is a particular example of a NEMS device, an exciting generation of electronic devices such as: sensitive mechanical charge detector, logic gates, sensors, and memories. Beside these applications, a charge shuttle may increase the understanding of quantum transport properties of NEMS and related quantum phenomena in

nanoscopic systems. In an original proposal for a charge shuttle by Gorelik, et al[20], the investigation of the quantization of charge in the strong Coulomb blockade regime was discussed. This system consists of a movable, micro-size metallic grain spatially confined in a harmonic potential between source and drain leads. In the strong Coulomb blockade regime only a single excess electron at a time is allowed to occupy the grain. When a sufficiently high bias is applied between the leads, a single electron may tunnel onto the grain, and due to the electrostatic field between the leads, the charged grain is driven towards the drain, where the electron tunnels off. Due to the harmonic potential the uncharged grain is forced back towards the source and the process is repeated. A mesoscopic shuttle system similar in some respects to that proposed by Gorelik et al. has been experimentally realized[12, 21]. This situation has been investigated both in the incoherent and in the quantum case. The shuttling phenomenon has been observed in Parks et al., experiment[7], where a  $C_{60}$  molecule is oscillating between two leads. In this experiment, Parks et al., have observed the quantization of current for various applied voltages, which exhibits step like features within the current-voltage (I-V) curve. The molecular shuttling between the electrodes in this experimental setup has been done at low amplitude and high frequency but provided a key evidence of the involvement of phonon levels in changing the current properties. This quantized behavior in the conductance characteristics of NEMS devices has been observed in a similar experiment[22]. Another method to drive the oscillations is to use an external AC electric field acting on a cantilever (Erbe et al.,)[12], where the amplitude can be tuned independently of the source-drain voltage bias. More recently[19], I-V characteristics of a quantum shuttle device have been observed at room temperature. These experiments are very close to the original proposal of Gorelik, et al.

In general, there are two different theoretical formulations that can be used to study the quantum transport in nanoscopic systems under voltage bias. Firstly,

a generalized quantum master equation approach[23–26] and secondly, the nonequilibrium Green’s function (NEGF)[27, 28] formulation. The former leads to a simple rate equation, where the coupling between the dot and the leads is considered as a weak perturbation and the electron-phonon interaction is also considered very weak. In the latter case one can consider strong leads to system and electron-phonon coupling. The nonequilibrium Green’s function technique is able to deal with a very broad variety of physical situations related to shuttling transport[30] at molecular[31] levels. It can deal with strong non-equilibrium situations and very small to very large applied bias. In the early seventies, the nonequilibrium Green’s function approach was applied to mesoscopic[32–35] transport by Caroli et al., where they were mainly interested in inelastic transport effects in tunneling through oxide barriers. This approach was formulated in an elegant way[28, 36–39] by Mier et al, where they have shown an exact time dependent expression for the non-equilibrium current through mesoscopic systems. In this model an interacting and non-interacting mesoscopic system was placed between two large semi-infinite leads. Furthermore, NEGF has been applied in the study of shot noise in chain models[40] and disordered junctions[41] while noise in Coulomb blockade Josephson junctions has been discussed within a phase correlation theory approach[42]. In the case of an inelastic resonant tunneling structure, in which strong electron-phonon coupling is often considered, a very strong source-drain voltage is expected for which coherent electron transport in molecular devices has been considered by some workers[43] within the scattering theory approach. Recently, phonon assisted resonant tunneling conductance has been discussed within the NEGF technique at zero temperature[44]. To the best of our knowledge, in all these studies, time-dependent transport properties via a quantum shuttle have not been discussed so far. The development of time-dependent quantum transport for the treatment of nonequilibrium system with phononic as well as Fermionic degrees of freedom has remained a challenge since the 1980’s[27, 28, 36–39, 45]. Generally, time-dependent transport properties of mesoscopic systems without an oscillating dot have been reported[46] and, in particular, sudden joining of the leads with a quantum dot or molecule have been investigated[45, 47] for the case of a noninteracting quantum dot and for a weakly Coulomb interacting molecular system. Strongly interacting systems in the Kondo regime have been investigated[48, 49]. More recently[50], the transient effects occurring in a molecular quantum dot described by an Anderson-Holstein Hamiltonian has been discussed.

In most of the theoretical work on shuttle based devices since the original proposal[20], mechanical degree of freedom has been described classically/semiclassically or quantum mechanically using the quantum master or rate equation approach[20, 23–26]. In the original proposal, the mechanical part was also treated classically, including

the damped oscillator, and assuming an incoherent electron tunneling process. This approach is based on a perturbation, weak coupling and large applied bias approximations, whereas the Keldysh nonequilibrium Green’s function formulation can treat the system-leads and electron-phonon coupling with strong interactions[51] for both small and large applied bias voltage. Moreover, the theories of the Jauho group[24] and Armour[23] fail to explain the low bias regime. The transport properties have been described and discussed semi-classically/classically but need a complete quantum mechanical description. A theory beyond these cases is required in order to further refine experiments on quantum shuttle based NEMS devices. In the quantum transport properties of a quantum shuttle; the quantized current can be determined by the frequency of the quantum mechanical oscillator, the interplay between the time scales of the electronic and mechanical degrees of freedom, and the suppression of stochastic tunneling events due to matching of the Fermionic and oscillator properties. For this reason, a first complete analytical and qualitative description of the quantum transport properties of a simple quantum shuttle device is performed and discussed in detail in this work.

In the present work, we shall investigate the time evolution of an oscillating quantum dot as a reaction to a sudden joining to the leads. We employ the nonequilibrium Green’s function method in order to discuss the transport properties of a quantum shuttle device. In this system, we include the time-dependent hopping between the oscillating dot and the leads to enable us to connect the leads to the dot at a finite time. An advantage of the time-dependent non-equilibrium Green’s function approach considered in this work is that it eliminates the one major criticism of the Keldysh approach, which is the lack of any clear initial conditions. We assume strong dissipation of the oscillating dot, where we consider the average over single particle properties, implicitly assuming strong damping of the mechanical oscillator. Simply averaging over a single particle expression is a valid description of a many particle problem, as long as any excitation caused by one electron has been dissipated before the next electron arrives. This is the strong dissipation regime. We describe the electronic state of the dot as a two-state system (empty/occupied). The electrons in the leads are considered to be at zero temperature. We consider an arbitrary finite chemical potential difference between the right and left leads. The transient and the steady state behavior of the system is considered here in order to explore the quantum dynamics of the shuttle device as a function of time. This is a fully quantum mechanical formulation whose basic approximations are very transparent, as the technique has already been used to study transport properties in a wide range of mesoscopic systems. In most of the existing literature very big chemical potential difference is considered while we include a range from very small to very large. In our calculation inclusion of the oscillator is not perturbative. As

the recent[16] studies are beyond the perturbation theory, a non-perturbative approach is required beyond the quantum master equation or linear response. Hence, our work provides an exact analytical solution to the current-voltage, correlation functions, average energy, coupling of leads with the system, very small chemical potential difference and includes both the right and left Fermi level response regimes. For simplicity, we used the wide-band approximation, where the density of states in the leads and hence the coupling between the leads and the dot was taken to be independent of energy. Although the method we used does not rely on this approximation. This provides a way to perform transient transport calculations from first principles while retaining the essential physics of the electronic structure of the dot and the leads. Another advantage of this method is that it treats the infinitely extended reservoirs in an exact way in the present system, which may give a better understanding of the essential features of charge shuttle based NEMS device in a more appropriate quantum mechanical picture.

## II. FORMULATION

The model consists of a moveable quantum dot suspended between the right and the left semi-infinite leads. This model is a close analogue to the dot attached to the tip of a cantilever or connected to the leads by some soft material or embedded into an elastic matrix. In this model the center of mass of the nanoparticle is confined to a harmonic potential. In the most recent experimental realizations of a quantum dot shuttle (QDS)[19] at room temperature, due to its small diameter, the quantum dot has a very small capacitance and thus has a charging energy that exceeds the thermal energy  $k_B T$ . Due to Coulomb blockade we consider only one excess electron can occupy the device. We consider the electronic state of the central quantum dot as empty or charged (a two level system). The tunneling amplitude of the electrons depends exponentially on the position of the central island and thus electrons can tunnel between the leads and the quantum dot. This is due to the exponentially decreasing/increasing overlapping of the electronic wave functions.

The coupled system is described by a single electronic level of energy  $\epsilon_0$  and a nanomechanical oscillator with frequency  $\omega$  and mass  $\mu$ . An electrostatic force ( $eE$ ) acts on the mechanical grain when the quantum dot is charged and gives the electrical influence on the nanomechanical dynamics of the system. The electric field  $E$  is generated by the voltage drop between the left and the right leads. In our model, though, it is kept as an external parameter. The quantum dynamics of the nanomechanical oscillator is represented in terms of position and momentum operators. In terms of creation and annihilation operators for the nanomechanical oscillator excitations the Hamiltonian of our simple system is[20, 23–25, 44, 52, 53]

$$H_0 = H_{\text{dot-ph}} + H_{\text{leads}} \quad (1)$$

$$H_{\text{dot-ph}} = [\epsilon_0 + \eta(b^\dagger + b)] c_0^\dagger c_0 + H_{ph}, \quad (2)$$

$$H_{ph} = \frac{\hat{p}^2}{2\mu} + \frac{1}{2}\mu\omega\hat{x}^2 = \hbar\omega(b^\dagger b + \frac{1}{2}), \quad (3)$$

where  $\epsilon_0$  is the single energy level of electrons on the dot with  $c_0^\dagger, c_0$  the corresponding creation and annihilation operators, and an oscillator of frequency  $\omega$ , mass  $\mu$  and  $b^\dagger, b$  are the raising and lowering operator of the phonons. The parameter  $\eta = \frac{\lambda l}{\sqrt{2}}$  physically represents an effective electric field in the capacitor seen by the moving dot between the leads, which we shall refer to as the coupling strength between the moving dot and the electrons on the dot given as  $\lambda l = eEl$ , where  $e$  is the charge of electron,  $E$  is the strength of electric field and  $l = \sqrt{\frac{\hbar}{\mu\omega}}$  is the zero point amplitude of the oscillator. The remaining elements of the Hamiltonian are

$$H_{\text{leads}} = \sum_k \epsilon_j c_j^\dagger c_j, \quad (4)$$

$$H_{\text{leads-dot}} = \Delta H_\alpha = \frac{1}{\sqrt{N}} \sum_j V_\alpha(t) (c_j^\dagger c_0 + c_0^\dagger c_j), \quad (5)$$

where  $N$  is the total number of states in the lead,  $\alpha = L, R$ , and  $j$  represents the channels in one of the leads. We include the time-dependent hopping  $V_\alpha(t)$  to enable us to connect the leads  $\alpha$  to the moving dot at a finite time. An advantage of this approach (joining of leads to the dot at  $t=0$ ) is that it eliminates the one major criticism of Keldysh approach, namely the lack of any clear initial conditions.  $V_\alpha(t)$  is written as

$$V_\alpha(t) = V_0(t) e^{\mp \xi \hat{x}} \quad (6)$$

where  $\xi = \frac{1}{\zeta}$  is the inverse tunneling length ( $\zeta$ ),  $-$  stands for  $V_L(t) = V_0(t) e^{-\xi \hat{x}}$  and  $+$  stands for  $V_R(t) = V_0(t) e^{+\xi \hat{x}}$ . For the time-dependent dynamics, we shall focus on sudden joining of the leads to the moving dot at  $t = 0$ , which means  $V_0(t) = V\theta(t)$ , where  $\theta(t)$  is the Heaviside unit step function. The displacement operator is given as

$$\hat{x} = \frac{l(b^\dagger + b)}{\sqrt{2}} \quad (7)$$

The total Hamiltonian of the system is thus  $H = H_0 + \Delta H_\alpha$ . We write the eigenvalues and the eigenfunctions of  $H_{\text{dot-ph}}$  as

$$\epsilon = \epsilon_0 + \hbar\omega(n + \frac{1}{2}) - \Delta \quad (8)$$

$$\Psi_m(K, x_0 \neq 0) = A_m \exp[-\frac{l^2 K^2}{2}] H_m(lK) \exp[-iKx_0] \quad (9)$$

$$\Psi_n(K, x_0 = 0) = A_n \exp[-\frac{l^2 K^2}{2}] H_n(lK), \quad (10)$$

for the occupied,  $x_0 \neq 0$  and unoccupied,  $x_0 = 0$ , dot respectively, where  $A_n = \frac{1}{\sqrt{\pi 2^n n! l}}$ ,  $A_m = \frac{1}{\sqrt{\pi 2^m m! l}}$ ,  $\Delta = \frac{\lambda^2}{2\mu\omega^2}$ ,  $x_0 = \frac{\lambda}{\mu\omega^2}$  is the displaced oscillator equilibrium position due to the coupling to the electrons on the dot, and  $H_n(lK)$  are the usual Hermite polynomials. Here we have used the fact that the harmonic oscillator eigenfunctions have the same form in both real and Fourier space.

In order to transform between the representations for the occupied and unoccupied dot we require the matrix with elements  $\Phi_{n,m} = \int \Psi_n^*(K, x_0 = 0) \Psi_m(K, x_0 \neq 0) dK$ , which may be simplified[54] as

$$\Phi \equiv \Phi_{n,m} = \sqrt{\frac{2^{|m-n|} \min[n, m]!}{\max[n, m]!}} \exp(-\frac{1}{4}x^2) \times (\frac{1}{2}ix)^{|m-n|} L_{\min[n, m]}^{|m-n|}(\frac{1}{2}x^2), \quad (11)$$

where  $x = \frac{x_0}{l}$  is the ratio of equilibrium position of the displaced oscillator to the zero point amplitude of the oscillator and  $L_n^{m-n}(x)$  are the associated Laguerre polynomials. The position of the resonant level with respect to the chemical potential in the leads is thus affected by  $x$  of the nanomechanical oscillator, which in turn affects the transport properties of the junction through the device.

### III. THE SELF-ENERGY AND THE GREEN'S FUNCTION

In order to calculate the analytical solutions and to discuss the numerical results of the transient and steady state quantum dynamics of the nanomechanical shuttle device, our focus in this section is to derive an analytical relation for the time-dependent effective self energy and the corresponding Green's function. The effective self-energy represents the contribution to the moving dot energy, due to interactions between the oscillating dot and the leads it is coupled to. In obtaining these results we use the wide-band approximation only for the simplicity, although the method we are using does not rely on this approximation. The retarded self-energy of the oscillating dot due to each lead is given by[28, 36–39, 45] (see Appendix)

$$\Sigma^r(t, t_1) = -\frac{i\Gamma_\alpha}{2} \theta(t_2) \delta(t - t_1) \Sigma^r(\mp) \quad (12)$$

with the matrix  $\Sigma^r(\mp)$

$$\begin{aligned} \Sigma^r(\mp) &\equiv \Sigma_{n_0, n'_0}^r(\mp) \\ &= \exp[(\gamma \mp x)^2 - x^2] \sqrt{\frac{2^{|n'_0 - n_0|} \min[n_0, n'_0]!}{\max[n_0, n'_0]!}} \\ &\quad \times (\mp \gamma)^{|n'_0 - n_0|} L_{\min[n_0, n'_0]}^{|n'_0 - n_0|}(-2\gamma^2), \end{aligned} \quad (13)$$

where  $\Sigma^a(t, t_1) = (\Sigma^r(t, t_1))^*$  with  $\alpha$  representing the L or R leads, the dimensionless tunneling length  $\gamma = \frac{\xi l}{\sqrt{2}}$ ,  $x = \frac{x_0}{l}$ , and the  $-$ ,  $+$  signs stands for the left and the right leads respectively. In the present representation, the effective self energy is given in terms of a matrix due to the position dependence of the tunneling matrix elements.

The final result for the lesser self energy matrix may be written as

$$\begin{aligned} \Sigma^<(t_1, t_2) &= i\Gamma_\alpha \theta(t_1) \theta(t_2) \times \Sigma^<(\mp) \\ &\quad \times \int_{-\infty}^{\epsilon_F \alpha + \frac{1}{2}\hbar\omega} \frac{d\varepsilon_\alpha}{2\pi} \exp[-i\varepsilon_\alpha(t_1 - t_2)], \end{aligned} \quad (14)$$

where the matrix element of the lesser self-energy is written as

$$\Sigma^<(\mp) = \mathbf{V}^<(\mp) [\mathbf{V}^<(\mp)]^\dagger, \quad (15)$$

where  $\mathbf{V}^<(\mp) \equiv V_n^<(\mp) = \frac{\exp[-\frac{x^2}{2} + (\frac{\gamma \mp x}{2})^2]}{\sqrt{n!}} [\mp(\frac{\gamma \pm x}{2})]^n$ .

This model represent the interplay between two physical time scales of the system, i.e., the oscillator frequency ( $\omega$ ), and the tunneling rate ( $\Gamma_\alpha$ ). The model also shows very interesting interplay between three physical length scales of the system, i.e., dimensionless tunneling length ( $\gamma$ ), zero point amplitude ( $l$ ) and the displaced oscillator equilibrium position to the zero point amplitude of the oscillator ( $x$ ), which are actually affected by the weak and strong coupling dynamics and small and large tunneling rate.

We solve Dyson's equation using  $H_{\text{dot-leads}}$ , as a perturbation in terms of matrix representation. In the presence of the oscillator, the matrix of the retarded,  $\mathbf{G}^r(t, t_1)$  and advanced,  $\mathbf{G}^a(t_2, t')$  Green's functions on the dot, with the phonon states may be written as

$$\begin{aligned} \mathbf{G}^r(t, t_1) &= -i\theta(t - t_1) \exp[-i(\mathbf{M})(t - t_1)], \quad t_1 > 0 \\ &\equiv G_{m, n_0}^r(t, t_1) \end{aligned} \quad (16)$$

where  $\mathbf{G}^r$  and  $\mathbf{M}$  are matrices in nanomechanical oscillator space with indices  $m, n_0$ , and the matrix  $\mathbf{M}$  may be written as

$$\mathbf{M} \equiv (E_m \delta_{m, n_0} + \Sigma_{m, n_0}^r), \quad E_m = \epsilon_0 + (m + \frac{1}{2})\hbar\omega - \Delta, \quad (17)$$

$$\begin{aligned} \mathbf{G}^a(t_2, t') &= (\mathbf{G}^r(t', t_2))^* \\ &= +i\theta(t' - t_2) \exp[-i(\mathbf{M}^*)(t_2 - t')], \quad t_2 > 0 \\ &\equiv G_{n', k}^a(t_2, t') \end{aligned} \quad (18)$$



The above Eqs. (12), (14), (16), and (18) will be the starting point of our examination of the time-dependent response of the coupled system. These functions are the essential ingredients for theoretical consideration of such diverse problems as low and high voltage, coupling of electron and phonons, transient and steady state phenomena.

#### IV. THE DENSITY MATRIX $\rho_{n,n'}(t, t)$ AND THE CORRELATION FUNCTION

The density matrix is related to the lesser Green's function through  $\rho_{n,n'}(t, t) = -iG_{n,n'}^<(t, t')$  at  $t' = t$ , where the  $G_{n,n'}^<(t, t')$  is the lesser Green's function[27, 28, 36–39, 45] on the oscillating dot including all the contribution from the leads. When  $t$  and  $t' > 0$  the lesser Green's function for the dot in the presence of the nanomechanical oscillator on the dot, with phonon states in the representation of the unoccupied dot, may be written as

$$\begin{aligned} G_{n,n'}^<(t, t') &= \sum_{m, n_0, n', k} \int_0^t \int_0^{t'} dt_1 dt_2 \\ &\times \Phi_{n,m} G_{m,n_0}^r(t, t_1) \Sigma_{n_0, n'}^<(t_1, t_2) G_{n', k}^a(t_2, t') \Phi_{n', k}^* \\ &\equiv \int_0^t \int_0^{t'} \Phi \mathbf{G}^r(t, t_1) \Sigma^<(t_1, t_2) \mathbf{G}^a(t_2, t') \Phi^\dagger dt_1 dt_2 \quad (19) \end{aligned}$$

whereas for  $t$  and  $t' < 0$ , the  $G_{n,n'}^<(t, t')$  is equal to zero.  $G_{n,n'}^<(t, t')$  includes all the information for the nanomechanical oscillator and electronic leads of the system, and  $m, k, n_0, n_1, n, n'$  are the oscillator indices. The lesser self-energy,  $\Sigma_{n_0, n_1}^<(t_1, t_2)$ , contains electronic and oscillator contributions. The electronic contributions are non-zero only when  $t_1$  and  $t_2 > 0$ . The retarded Green's function,  $G_{m, n_0}^r(t, t_1)$ , is represented as

$$\mathbf{G}^r(t, t_1) = -i\theta(t - t_1) \exp[-i(\mathbf{M})(t - t_1)], \quad (20)$$

Using the eigenvalues and eigenfunctions of  $\mathbf{M}$ , the retarded Green's function may be written as

$$\mathbf{G}^r(t, t_1) = \mathbf{U} \mathbf{g}^r(t, t_1) \mathbf{U}^\dagger, \quad (21)$$

with eigenvectors  $\mathbf{U}$  and its inverse such that  $\mathbf{U} \mathbf{U}^\dagger = \mathbf{I}$  (not  $\mathbf{U} \mathbf{U}^\dagger = \mathbf{I}$ ), and

$$\begin{aligned} \mathbf{g}^r(t, t_1) &\equiv g_i^r(t, t_1) \\ &= -i\theta(t - t_1) \exp[-i(\epsilon_i - i\zeta_i)(t - t_1)] \delta_{i,j}, \quad (22) \end{aligned}$$

where  $\epsilon_i, \zeta_i$  are the real and imaginary parts of the  $i$ th eigenvalue of the matrix  $\mathbf{M}$ . The advanced Green's function,  $G_{n_1, k}^a(t_2, t)$ , is written as

$$\mathbf{G}^a(t_2, t') = +i\theta(t' - t_2) \exp[-i(\mathbf{M}^*)(t_2 - t')], \quad (23)$$

In terms of eigenvalues and eigenfunctions, the advanced Green's function is written as

$$\mathbf{G}^a(t_2, t') = \mathbf{U}^* \mathbf{g}^a(t_2, t') \mathbf{U}^\dagger, \quad (24)$$

with eigenvectors  $\mathbf{U}^*$  and its inverse such that  $\mathbf{U}^* \mathbf{U}^\dagger = \mathbf{I}$ , and

$$\begin{aligned} \mathbf{g}^a(t_2, t') &\equiv g_i^a(t_2, t') \\ &= +i\theta(t' - t_2) \exp[-i(\epsilon_i + i\zeta_i)(t_2 - t')] \delta_{i,j}, \quad (25) \end{aligned}$$

The lesser self-energy,  $\Sigma^<(t_1, t_2)$ , in matrix space of the oscillator was derived in the previous section.

The lesser Green's function can be calculated by using Eqs. (14, 21, & 24) in equation (19) at  $t = t'$  as

$$\begin{aligned} G_{n,n'}^<(t, t) &\equiv \int_0^t \int_0^t dt_1 dt_2 \Phi \mathbf{U} \mathbf{g}^r(t, t_1) \mathbf{U}^\dagger \Sigma^<(t_1, t_2) \mathbf{U}^* \mathbf{g}^a(t_2, t) \mathbf{U}^\dagger \Phi^\dagger, \\ &= \int_0^t \int_0^t dt_1 dt_2 \sum_{g, b, \alpha} [\Phi \mathbf{U}]_{n, g} \mathbf{g}^r(t, t_1) \mathbf{U}^\dagger \\ &\times \Sigma^<(\mp) \Sigma_\alpha^<(t_1, t_2) \mathbf{U}^* \mathbf{g}^a(t_2, t) [\Phi \mathbf{U}]_{b, n'}^\dagger, \\ &= \sum_{g, b, \alpha} [\Phi \mathbf{U}]_{n, g} [\mathbf{U}^\dagger \Sigma^<(\mp) \mathbf{U}^*]_{g, b} \chi_{g, b}^\alpha(t) [\Phi \mathbf{U}]_{b, n'}^\dagger, \quad (26) \end{aligned}$$

where the function  $\chi_{g, b}^\alpha(t)$  is written as

$$\chi_{g, b}^\alpha(t) = \int_0^t \int_0^t dt_1 dt_2 g_g^r(t, t_1) \Sigma_\alpha^<(t_1, t_2) g_b^a(t_2, t) \quad (27)$$

which can be written as

$$\begin{aligned} \chi_{g, b}^\alpha(t) &= \int_0^t \int_0^t dt_1 dt_2 \exp[-i(\epsilon_g - i\zeta_g)(t - t_1)] \\ &\times \left\{ i\Gamma_\alpha \int_{-\infty}^{\epsilon_{F\alpha} + \frac{1}{2}\hbar\omega} \frac{d\varepsilon_\alpha}{2\pi} \exp[-i\varepsilon_\alpha(t_1 - t_2)] \right\} \\ &\times \exp[-i(\epsilon_b + i\zeta_b)(t_2 - t)], \quad (28) \end{aligned}$$

Although  $\mathbf{G}^{r(a)}(t, t')$  is non-zero for  $t < 0$ , it is never required due to the way it combines with  $\Sigma_\alpha^{r(a), (<)}(t, t')$ . By carrying out the time integrations, the resulting expression is written as

$$\begin{aligned} \chi_{g, b}^\alpha(t) &= \frac{i\Gamma_\alpha}{2\pi} \int_{-\infty}^{\epsilon_{F\alpha} + \frac{1}{2}\hbar\omega} d\varepsilon_\alpha \frac{1}{(\varepsilon_\alpha - \epsilon_b - i\zeta_b)(\varepsilon_\alpha - \epsilon_g + i\zeta_g)} \\ &\times \left\{ 1 + \exp[i(\epsilon_b - \epsilon_g + i(\zeta_b + \zeta_g))t] \right. \\ &\quad - \exp[-i(\varepsilon_\alpha - \epsilon_b - i\zeta_b)t] \\ &\quad \left. - \exp[i(\varepsilon_\alpha - \epsilon_g + i\zeta_g)t] \right\} \quad (29) \end{aligned}$$

For all values of  $b, g$ , and  $\alpha$ ,  $\chi_{g,b}^\alpha(t=0)$  must be equal to zero. The integral over the energy in the above equation is carried out[55]. The final result for the above expression is written as

$$\chi_{g,b}^\alpha(t) = \frac{i\Gamma_\alpha}{2\pi} \left\{ \frac{1}{\varepsilon_b - \varepsilon_g + i(\zeta_b + \zeta_g)} \right\} [Y_{g,b}^\alpha + Z_{g,b}^\alpha], \quad (30)$$

where we have added the contribution from the right and the left leads, which can be written in terms of  $\alpha$  as

$$\begin{aligned} Y_{g,b}^\alpha &= (1 + \exp[i(\varepsilon_b - \varepsilon_g + i(\zeta_b + \zeta_g))t]) \\ &\times \left\{ \frac{1}{2} \frac{\ln[(\epsilon_{F\alpha} - \varepsilon_b)^2 + \zeta_b^2]}{\ln[(\epsilon_{F\alpha} - \varepsilon_g)^2 + \zeta_g^2]} \right. \\ &\quad + i \left[ \tan^{-1} \left( \frac{\varepsilon_{F\alpha} - \varepsilon_b}{\zeta_b} \right) \right. \\ &\quad \left. \left. + \tan^{-1} \left( \frac{\varepsilon_{F\alpha} - \varepsilon_g}{\zeta_g} \right) + \pi \right] \right\}, \quad (31) \end{aligned}$$

and

$$\begin{aligned} Z_{g,b}^\alpha &= \exp[i(\varepsilon_b - \varepsilon_g + i(\zeta_b + \zeta_g))t] \\ &\times (-\text{Ei}[it(\epsilon_{F\alpha} - \varepsilon_b - i\zeta_b)] + \text{Ei}[-it(\epsilon_{F\alpha} - \varepsilon_g + i\zeta_g)]) \\ &+ \text{Ei}[it(\epsilon_{F\alpha} - \varepsilon_g + i\zeta_g)] - \text{Ei}[-it(\epsilon_{F\alpha} - \varepsilon_b - i\zeta_b)], \quad (32) \end{aligned}$$

with  $\epsilon_{F\alpha}$  being the right and the left Fermi levels and  $\text{Ei}(x)$  the exponential integral function. Special care is required in evaluating the  $\text{Ei}(x)$  to choose the correct Riemann sheets in order to make sure that these functions are consistent with the initial conditions  $\chi_{g,b}^\alpha(t=0) = 0$  and are continuous functions of time and chemical potential for each value of  $b, g$ , and  $\alpha$ .

Now using equation (26), the dot population may be written as

$$\rho(t) = \sum_n \rho_{n,n}^<(t, t) = \sum_n -iG_{n,n}^<(t, t), \quad (33)$$

Next we derive a relation for the correlation function which is an interesting physical quantity to see the shuttling dynamics of the system. With the help of equation (26) the correlation function  $\text{Tr} \langle \hat{p} \mathbf{G}^<(t, t) \rangle$ , where  $\hat{p} = \frac{i\mu\omega}{\sqrt{2}}(b^\dagger - b)$  is the momentum operator of the oscillator, may be written as

$$\begin{aligned} &\text{Tr} \left\langle \frac{i\mu\omega}{\sqrt{2}} (b^\dagger - b) \mathbf{G}^<(t, t) \right\rangle \\ &= \sum_n \left\langle \frac{i\mu\omega\sqrt{n}}{\sqrt{2}} \{G_{n-1,n}^<(t, t) - G_{n,n-1}^<(t, t)\} \right\rangle, \quad (34) \end{aligned}$$

which we expect to be finite in case of shuttling as the dot should be occupied for positive momentum while zero for unoccupied dot. As we note that the momentum correlation function depends on off-diagonal elements of the lesser Green's function which can only be finite when nanomechanical oscillator is in a mixed quantum state rather than in a simple eigenstate.

## V. TIME-DEPENDENT CURRENT FROM LEAD $\alpha$

The particle current  $I_\alpha$  into the interacting region from the lead is related to the expectation value of the time derivative of the number operator  $N_\alpha = \sum_{\alpha j} c_{\alpha j}^\dagger c_{\alpha j}$ , as[28, 36–39, 45–47]

$$I_\alpha = -e \left\langle \frac{d}{dt} x \right\rangle = \frac{ie}{\hbar} \langle [x, H] \rangle$$

and the final result for the current through each of the leads is written as (See Ref. 51 for detail) as

$$\begin{aligned} I_\alpha(t) &= \frac{e}{\hbar} \int_0^t dt_1 \\ &\times \text{Tr} \{ \mathbf{G}^r(t, t_1) \mathbf{\Sigma}^<(t_1, t) + \mathbf{G}^<(t, t_1) \mathbf{\Sigma}^a(t_1, t) \\ &\quad - \mathbf{\Sigma}^r(t, t_1) \mathbf{G}^<(t_1, t) - \mathbf{\Sigma}^<(t, t_1) \mathbf{G}^a(t_1, t) \}, \\ &= \frac{e}{\hbar} (Z_1^\alpha + Z_2^\alpha) \quad (35) \end{aligned}$$

where  $Z_1^\alpha$  is defined as

$$\begin{aligned} Z_1^\alpha &\equiv \int_0^t dt_1 \text{Tr} \{ \mathbf{G}^r(t, t_1) \mathbf{\Sigma}^<(t_1, t) - \mathbf{\Sigma}^<(t, t_1) \mathbf{G}^a(t_1, t) \} \\ &= \int_0^t dt_1 \text{Tr} \{ \mathbf{U} \mathbf{g}^r(t, t_1) \mathbf{U}^\dagger \mathbf{\Sigma}^<(\mp) \mathbf{\Sigma}_\alpha^<(t_1, t) \\ &\quad - \mathbf{\Sigma}^<(\mp) \mathbf{\Sigma}_\alpha^<(t, t_1) \mathbf{U}^* \mathbf{g}^a(t_1, t) \mathbf{U}^\dagger \} \\ &= \sum_g \{ [\mathbf{U}^\dagger \mathbf{\Sigma}^<(\mp) \mathbf{U}]_{g,g} \chi_g^\alpha(t) \\ &\quad - \sum_g [\mathbf{U}^\dagger \mathbf{\Sigma}^<(\mp) \mathbf{U}^*]_{g,g} (\chi_g^\alpha(t))^* \}, \quad (36) \end{aligned}$$

where  $\chi_g^\alpha(t)$  is defined as

$$\begin{aligned} \chi_g^\alpha(t) &= \int_0^t dt_1 g_g^r(t, t_1) \Sigma_\alpha^<(t_1, t) \\ &= \frac{-i\theta(t-t_1)}{2\pi} \int_0^t dt_1 \exp[-i(\epsilon_g - i\zeta_g)(t-t_1)] \\ &\quad \times i\Gamma_\alpha \int_{-\infty}^{\epsilon_{F\alpha} + \frac{1}{2}\hbar\omega} d\varepsilon_\alpha \exp[-i\varepsilon_\alpha(t_1-t)] \\ &= \frac{i\Gamma_\alpha}{2\pi} \int_{-\infty}^{\epsilon_{F\alpha} + \frac{1}{2}\hbar\omega} d\varepsilon_\alpha \frac{1 - \exp[-i(\varepsilon_\alpha - \epsilon_g + i\zeta_g)t]}{\varepsilon_\alpha - \epsilon_g + i\zeta_g} \\ &= \frac{i\Gamma_\alpha}{2\pi} \{ \ln[(\epsilon_{F\alpha} - \varepsilon_g) + i\zeta_g] - \text{Ei}[it(\epsilon_{F\alpha} - \varepsilon_g + i\zeta_g)] \} \quad (37) \end{aligned}$$

Hence, the final result for  $Z_1^\alpha$  is written as

$$Z_1^\alpha = \frac{i\Gamma_\alpha}{2\pi} \left\{ \sum_g [\mathbf{U}^\dagger \Sigma^<(\mp) \mathbf{U}]_{g,g} \right. \\ \left. \times \left\{ \frac{1}{2} \ln[(\epsilon_{F\alpha} - \epsilon_g) + i\zeta_g] - \text{Ei}[it(\epsilon_{F\alpha} - \epsilon_g + i\zeta_g)] \right\} \right. \\ \left. - \text{c.c.} \right\} \quad (38)$$

and  $Z_2^\alpha$  is written as

$$\begin{aligned} Z_2^\alpha &\equiv \int dt_1 \text{Tr} \{ \mathbf{G}^<(t, t_1) \Sigma^a(t_1, t) - \Sigma^r(t, t_1) \mathbf{G}^<(t_1, t) \} \\ &= \int dt_1 \text{Tr} \left\{ \mathbf{G}^<(t, t_1) \Sigma^a(\mp) \frac{i\Gamma_\alpha}{2} \theta(t_1) \delta(t - t_1) \right. \\ &\quad \left. + \Sigma^r(\mp) \frac{i\Gamma_\alpha}{2} \theta(t_1) \delta(t - t_1) \mathbf{G}^<(t_1, t) \right\} \\ &= \text{Tr} \left\{ \frac{i\Gamma_\alpha}{2} \mathbf{G}^<(t, t) \Sigma^a(\mp) + \frac{i\Gamma_\alpha}{2} \Sigma^r(\mp) \mathbf{G}^<(t, t) \right\} \\ &= i\Gamma_\alpha \int_0^t \int_0^t dt_2 dt_3 \\ &\quad \text{Tr} \{ \mathbf{G}^r(t, t_3) \Sigma^<(\mp) \Sigma_\alpha^<(t_3, t_2) \mathbf{G}^a(t_2, t) \Sigma^a(\mp) \} \\ &= i\Gamma_\alpha \int_0^t \int_0^t dt_2 dt_3 \\ &\quad \text{Tr} \{ \mathbf{U} \mathbf{g}^r(t, t_3) \mathbf{U}^\dagger \Sigma^<(\mp) \Sigma_\alpha^<(t_3, t_2) \mathbf{U}^* \mathbf{g}^a(t_2, t) \mathbf{U}^\dagger \Sigma^a(\mp) \} \\ &= i\Gamma_\alpha \left\{ \sum_{g,b,\alpha} [[\mathbf{U}^\dagger \Sigma^a(\mp) \mathbf{U}]_{b,g} [\mathbf{U}^\dagger \Sigma^<(\mp) \mathbf{U}^*]_{g,b} \chi_{g,b}^\alpha(t)] \right\}, \end{aligned} \quad (39)$$

where  $\chi_{g,b}^\alpha(t)$  is as in (30).

Now using Eqs. (30, 38, & 39) in equation (35), we arrive at the final result for the current through lead  $\alpha$  as

$$I_\alpha(t) = \frac{e}{\hbar} (Z_1^\alpha + Z_2^L + Z_2^R), \quad (40)$$

where in calculating the left current we need  $Z_1^L$  and both the contributions  $Z_2^L$  and  $Z_2^R$  and for the right current  $Z_1^L$  is replaced by  $Z_1^R$ . As before, special care is required in evaluating the  $\ln(x)$  and  $\text{Ei}(x)$  to choose the correct Riemann sheets in order to make sure that these functions are consistent with the initial conditions  $I_\alpha(t) = 0$  and are continuous functions of time and chemical potential.

## VI. AVERAGE ENERGY

To calculate the energy transferred from the electrons to the nanomechanical oscillator, we return to the density matrix  $\rho_{n,n}(t, t)$  given in Eq. (33). We may use the lesser Green's function or density matrix to calculate the energy transferred to the oscillator as

$$E_{Ph} = \langle n \rangle \hbar\omega = \frac{\hbar\omega \sum_n n \rho_{n,n}(t, t)}{\sum_n \rho_{n,n}(t, t)} \quad (41)$$

where the average evaluated using the diagonal element of the density matrix on the oscillating quantum dot. Note that the normalization in equation (42) is required as the bare density matrix contains both electronic and oscillator contributions. The trace eliminates the oscillator part, leaving the electronic part.

## VII. DISCUSSION OF RESULTS

The net  $(I_L(t) - I_R(t))$  average current through the system, the correlation function  $\langle \hat{p} G^<(t, t) \rangle$ , total  $(I_L(t) + I_R(t))$  average current into the system, and the average energy of an oscillating dot between the leads are shown graphically as a function of time  $(2\pi/\omega)$  for different values of tunneling length, tunneling rate, and voltage bias. The following parameters were employed: the single energy level of the dot  $\epsilon_0 = 0.5$  and  $\epsilon_{FR} = 0$ . These parameters will remain fixed for all further discussions and have same dimension as  $\hbar\omega$ . We are interested in small and large values of tunneling rates  $(\Gamma_{L/R})$  from the leads, different values of the tunneling length  $(\zeta)$  between the oscillating dot and the electrons, and of the left chemical potential  $0 \leq \epsilon_{FL} \leq 2$ . The oscillating dot induced resonance effects are clearly visible in the numerical results. The tunneling rate of the electrons between the leads and the dot is considered to be asymmetric  $(\Gamma_R = \Gamma_L \exp[-\gamma x])$  and we assume that the leads have constant density of states. The values of the tunneling rates has been chosen such that when the dot is occupied and the zero point has moved to  $x_0$ , these values are reversed.

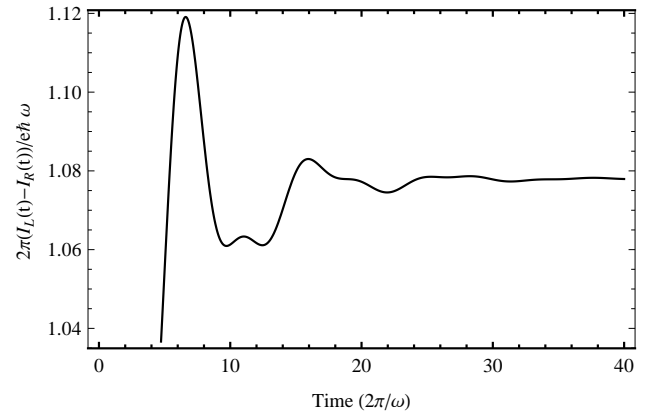


FIG. 1: Time-dependent net average current  $2\pi(I_L(t) - I_R(t))/e\hbar\omega$  against time  $(2\pi/\omega)$  for fixed values of the parameters:  $\epsilon_0 = 0.5$ ,  $\epsilon_{FR} = 0$ ,  $\epsilon_{FL} = 2$ ,  $x_0 = 0.2l$ ,  $\hbar\omega = 0.63$ ,  $\Gamma_L = \hbar\omega/2\pi$ ,  $\Gamma_R = \Gamma_L \exp[-\gamma x]$  and  $\gamma = 0.5$ . The electron per cycle behavior in this figure corresponds to the shuttling mechanism. Units: all the parameters have same dimension as of  $\hbar\omega$ .

In Fig. 1 & 2 we have shown the net average current  $2\pi(I_L(t) - I_R(t))/e\hbar\omega$  flowing through the system as a

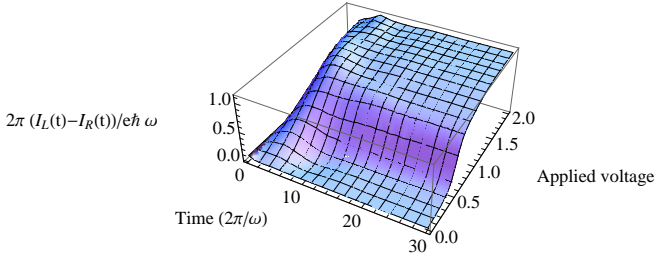


FIG. 2: Net average current  $(2\pi(I_L(t) - I_R(t))/e\hbar\omega)$  flowing through the system as a function of both time  $(2\pi/\omega)$  and of the left Fermi level for same values of the parameters as in fig. 1.

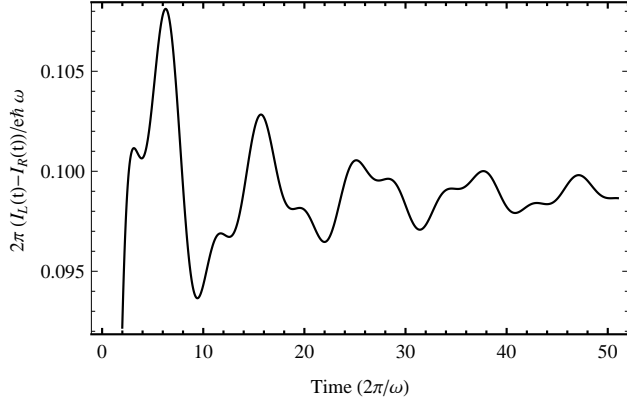


FIG. 3: Net average current  $(2\pi(I_L(t) - I_R(t))/e\hbar\omega)$  flowing through the system as a function of time  $(2\pi/\omega)$  for fixed values of the parameters in case of the tunneling mechanism:  $\epsilon_0 = 0.5, \epsilon_{FR} = 0, \epsilon_{FL} = 2, \hbar\omega = 0.63, \Gamma_L = \Gamma_R = 0.1\hbar\omega/2\pi, x_0 = 0.1l$  and  $\gamma = 0.001$ . Units: all the parameters have same dimension as of  $\hbar\omega$ .

function of time  $(2\pi/\omega)$  for fixed values of the Fermi level,  $\epsilon_{FL} = 2, \epsilon_{FR} = 0$ , tunneling energy,  $\Gamma_L = \hbar\omega/2\pi$ , the characteristic energy of the oscillator  $\hbar\omega = 0.63$ ,  $\Gamma_R = \Gamma_L \exp[-\gamma x]$ ,  $x_0 = 0.3l$  and finite  $\gamma = 0.5$ . This ( $\gamma = 0.5$ ) is the physical condition for shuttling in the quantum regime: when the zero point amplitude of the nanomechanical oscillator is half of the tunneling length ( $\zeta = \xi^{-1}$ ). In this figure, in which the oscillator period is comparable with the left bare tunneling rate ( $\Gamma_L = \hbar\omega/2\pi$ ), the average current saturates at one electron per mechanical cycle (corresponding to average current  $2\pi(I_L(t) - I_R(t))/e\hbar\omega = 1$ ) as the electrons are shuttled one by one from the source to the drain by the oscillating dot. We get the following physical picture: every time an electron jumps onto the dot when  $\Gamma_L = \hbar\omega/2\pi$ , the dot is near the source lead and subject to the electrostatic force  $eE$  that accelerates it towards the drain lead. Energy is pumped into the nanomechanical oscillator and the dot starts to oscillate between the leads. When the right tunneling time is high compared to the left tunnelling time, the oscillator dissipates this energy into the environment before the next event occurs.

This continuously drives the oscillator away from equilibrium and a stationary state is reached only when the energy pumped per cycle into the system is dissipated during the same cycle in the environment. With this setup, the system will be in the shuttle regime. We note that the frequency of the short period weak oscillations is  $(|\epsilon_{FL} - \epsilon_0|)$  and these oscillations are present even in the limit of small but finite  $\gamma$ . We conclude that this is a purely electronic process (plasmon oscillations). It is clear from the figure that in the strong tunneling case, it contains two beating frequencies, therefore we interpret this as due to a mixture of electronic and mechanical frequencies. In Fig. 2 the long time behavior of the net average current has steps as function of the left Fermi energy which become more pronounced with increasing  $\gamma$ . In contrast, when both the bare tunneling rates are equal and smaller than the mechanical frequency, and  $\gamma \ll 1$ , the dynamics of the system is similar to a double barrier resonant tunneling system, since the dot is static and far from both the leads. The tunneling dynamics of the net average current is shown in Fig. 3 for fixed values of  $\Gamma_L = \Gamma_R = 0.1\hbar\omega/2\pi, x_0 = 0.1l$  and the oscillator energy  $\hbar\omega = 0.63$ . This confirms the tunneling behavior of the system oscillating with beating frequency which is due to mixture of electronic and nanomechanical degrees of freedom and is consistent with previous studies[51].

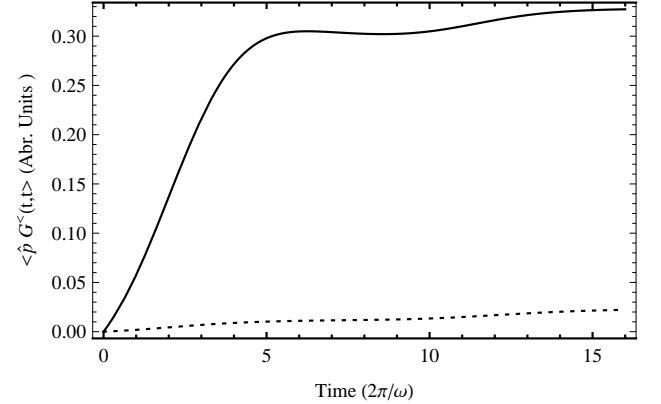


FIG. 4: The momentum correlation function as a function of time  $(2\pi/\omega)$  showing the shuttling (solid line) and the tunneling (dotted line) behavior. Parameters for the shuttling are  $\epsilon_0 = 0.5, \hbar\omega = 0.63, \Gamma_L = \hbar\omega/2\pi, x_0 = 0.2l, \Gamma_R = \Gamma_L \exp[-\gamma x]$  and  $\gamma = 0.5$ , and for the tunneling are  $\epsilon_0 = 0.5, \epsilon_{FR} = 0, \epsilon_{FL} = 2, \hbar\omega = 0.63, \Gamma_L = \Gamma_R = 0.1\hbar\omega/2\pi, x_0 = 0.1l$  and  $\gamma = 0.001$ . All the parameters have same dimension as  $\hbar\omega$ .

The correlation function is shown in Fig. 4 & 5, as a function of time  $(2\pi/\omega)$  and left Fermi energy for fixed values of tunneling length  $\zeta = 2l, x_0 = 0.5l, \hbar\omega = 0.63$  and tunneling rates  $\Gamma_L = \hbar\omega/2\pi, \Gamma_R = \Gamma_L \exp[-\gamma x]$ . We distinguish between the shuttling and tunneling dynamics of the system for long time for different tunneling rates and  $\gamma$ : For shuttling (solid line)  $\Gamma_L = \hbar\omega/2\pi, \Gamma_R = \Gamma_L \exp[-\gamma x], \gamma = 0.5$ , and for tunneling (dotted

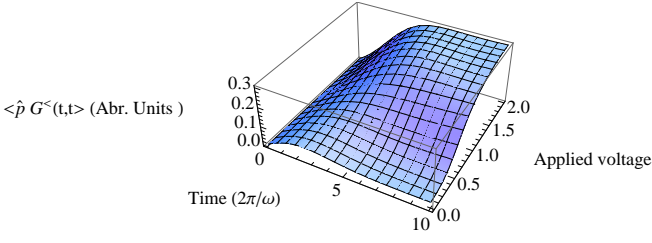


FIG. 5: The momentum correlation function as a function of time  $(2\pi/\omega)$  and left Fermi energy showing the shuttling behavior. Parameters for the shuttling are  $\epsilon_0 = 0.5$ ,  $\hbar\omega = 0.63$ ,  $\Gamma_L = \hbar\omega/2\pi$ ,  $x_0 = 0.2l$ ,  $\Gamma_R = \Gamma_L \exp[-\gamma x]$  and  $\gamma = 1$ . All the parameters have same dimension as of  $\hbar\omega$ .

line)  $\Gamma_L = \Gamma_R = 0.1\hbar\omega/2\pi$ ,  $x_0 = 0.1l$ , and  $\gamma = 0.001$ . Why have we found this particular type of structure? We know that, in the ideal shuttling regime, we expect the dot to be occupied when the momentum is positive and unoccupied when the momentum is negative. Hence, the correlation function is positive. In contrast, when the transport is independent of the mechanical oscillator, the correlation function is zero as  $\langle \hat{p} G^<(t,t) \rangle = \langle \hat{p} \rangle \langle G^<(t,t) \rangle = 0$ . We observe that the long time value of the correlation function has steps as a function of the left Fermi level as shown in fig. 5.

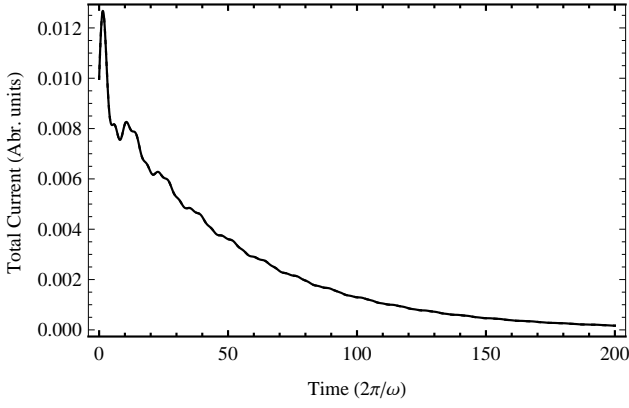


FIG. 6: Total average current  $(I_L(t) + I_R(t))$  flowing onto the dot as a function of time  $(2\pi/\omega)$  for fixed values of  $\epsilon_0 = 0.5$ ,  $\epsilon_{FR} = 0$ ,  $\epsilon_{FL} = 2$ ,  $\hbar\omega = 0.63$ ,  $\Gamma_L = \Gamma_R = 0.1\hbar\omega/2\pi$ ,  $x_0 = 0.2l$  and  $\gamma = 0.1$ . All the parameters have same dimension as  $\hbar\omega$ . This current (solid line) is equivalent to the rate of change of dot population  $\frac{d}{dt}\rho(t)$  (dashed line) as a function of time for same parameters as of current. In this figure, solid and dashed lines have same values at all points. Units: all the parameters have same dimension as of  $\hbar\omega$ .

Next, we have shown the total average current  $(I_L(t) + I_R(t))$  flowing onto the oscillating dot in Fig. 6 as a function of time  $(2\pi/\omega)$  for fixed values of  $\Gamma_L = \Gamma_R = 0.1\hbar\omega/2\pi$ ,  $\hbar\omega = 0.63$ ,  $\epsilon_{FR} = 0$ ,  $\epsilon_{FL} = 2$ , and finite value of the tunneling length  $\gamma = 0.1$ . This current (solid line) is equivalent to the rate of change of the dot population

(dashed line) for the same parameters. In this figure, we can not distinguish the solid and the dashed line. This confirms that our analytical results are consistent with the equation of continuity,  $I_L(t) + I_R(t) = \frac{d}{dt}\rho(t)$ , and hence, with the conservation laws for all parameters. We interpret the long period oscillations as a function of time  $(2\pi/\omega)$  is the mechanical frequency of the system and short period weak oscillations with the electronic frequency  $(|\epsilon_{FL} - \epsilon_0|)$ , which is consistent with the net average current results as well.

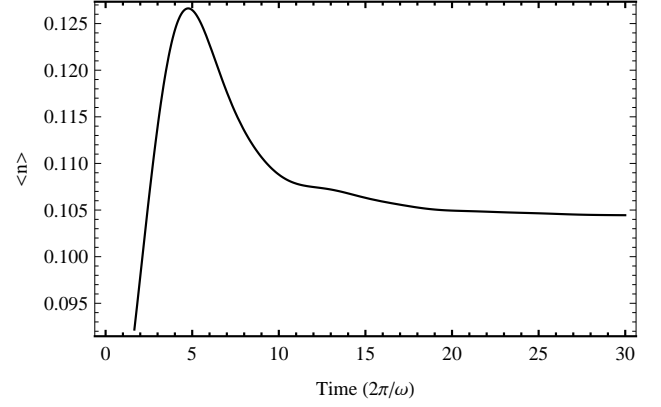


FIG. 7: Average energy transferred to the oscillator as a function of time  $(2\pi/\omega)$  for fixed values of  $\hbar\omega = 0.63$ ,  $\Gamma_L = \hbar\omega/2\pi$ ,  $x_0 = 0.5l$ ,  $\Gamma_R = \Gamma_L \exp[-\gamma x]$  and  $\gamma = 1$ . Units: all the parameters have same dimension as of  $\hbar\omega$ .

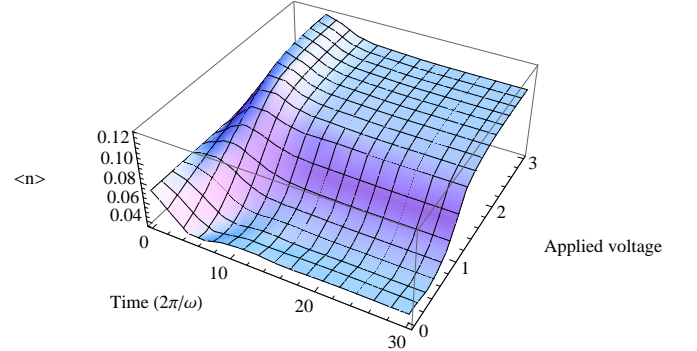


FIG. 8: Average energy transferred to the oscillator as a function of time  $(2\pi/\omega)$  and left Fermi energy for all the parameters same as in fig. 7.

Finally we have shown the average energy of the nanomechanical oscillator as a function of time  $(2\pi/\omega)$  and of the left Fermi energy in Fig. 7 & 8 for fixed values of tunneling rates  $\Gamma_L = 0.1$ ,  $\Gamma_R = \Gamma_L \exp[-\gamma x]$ ,  $\epsilon_{FR} = 0$ ,  $x_0 = 0.3l$  and tunneling length  $\gamma = 0.5$ . These parameters corresponds to the shuttling regime of the system. We found constant average energy of the nanomechanical oscillator for long time. This constant average energy increases with increasing Fermi level as shown in fig. 8. We consider two possible interpretations of this

structure. One is presented in the previous work: that the oscillator is in any of its pure states and therefore the potential seen by the electrons is time independent. Secondly, this is an average over several time-dependent processes with different phases such that any Rabi like features cancel. Hence, we note that only the second interpretation is consistent with the correlation function. For the case of the tunneling regime of the system, the average energy of the nanomechanical oscillator is shown in Fig. 9 as a function of time ( $2\pi/\omega$ ) for fixed values  $\Gamma_L = \Gamma_R = 0.1\hbar\omega/2\pi$ ,  $\hbar\omega = 0.63$ ,  $\epsilon_{FR} = 0$ ,  $\epsilon_{FL} = 2$ , and for very small value of the tunneling length  $l = 0.001\zeta$ .

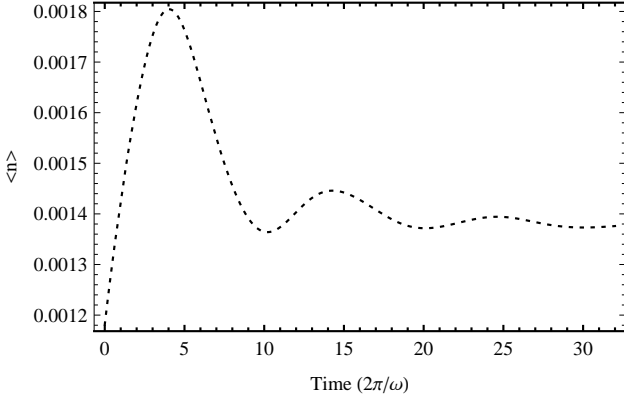


FIG. 9: Average energy transferred to the oscillator as a function of time ( $2\pi/\omega$ ) for fixed values of  $\epsilon_0 = 0.5$ ,  $\epsilon_{FR} = 0$ ,  $\epsilon_{FL} = 1$ ,  $\hbar\omega = 0.63$ ,  $\Gamma_L = \Gamma_R = 0.1\hbar\omega/2\pi$ ,  $x_0 = 0.5l$  and  $\gamma = 0.001$ . Units: all the parameters have same dimension as of  $\hbar\omega$ .

In Fig. 7, 8 & 9 it appears that the oscillator is not in its ground state at  $t=0$ . However, if we look at the structure of the lesser self-energy, the quantity in the middle refers to the state of the oscillator when the dot is empty and the oscillator is in its ground state. Whereas the whole self-energy refers to the state of the oscillator when an electron has passed through the barrier onto the dot. At this point the oscillator is not necessarily in its ground state. When the electron is in the leads, the oscillator is in its ground state but when the electron is on the dot two things happen: the representation of the lesser self-energy is changed and the other is the effect of the  $\exp[\mp\gamma x]$  operator which kicks the oscillator out of its ground state. This comes back into a saturated state for long time with finite value of average energy. This could be a mixed or a thermal state. When taken with the finite correlation function for the same parameters, we conclude that the long time average energy of the nanomechanical oscillator corresponds to the mixed state.

### VIII. SUMMARY

In this work, we analyzed the time-dependent transport via a quantum shuttle by using the nonequilibrium

Green's function approach without treating the electron phonon coupling as a perturbation. We have derived an expression for the full density matrix and discuss it in detail for different values of the tunneling length and the tunneling rate. Using the full density matrix calculation we have shown the oscillator momentum charge density correlation function which distinguishes the shuttling and the tunneling regime of the system. We derive an expression for the current to see the effects of the coupling of the electrons to the oscillator on the dot and the tunneling rate of electrons to resolve the dynamics of the nanomechanical oscillator. We found a positive correlation function for the nanomechanical oscillator in the shuttling regime and zero in the case of the tunneling regime. The shuttling regime will occur when the electron left jump rate introduces continued kicks on the island. This happens when the left jump rate is close to the oscillation frequency of the island  $\Gamma_L = \hbar\omega/2\pi$ . By setting an appropriate ejection rate ( $\Gamma_R = \Gamma_L \exp[-\gamma x]$ ) and  $l = 0.5\zeta$ , there exists a condition where the island will keep oscillating between the leads. In contrast, in the limit of equal bare tunneling rates, smaller than the mechanical frequency, and when  $\gamma \ll 1$ , the dynamics of the system is similar to a double barrier resonant tunneling system, where we found periodic oscillations as a function of time ( $2\pi/\omega$ ), which corresponds to the mechanical frequency of the system. Furthermore, we discuss the average energy transferred to oscillator as a function of time. We have found a mixed or a thermal state shown in the average energy of the nanomechanical oscillator for long time which is consistent with the finite correlation function for the same parameters. These results suggest further experiments for NEMS to go beyond the classical dynamics of a shuttle device.

### Appendix A:

In this appendix we derive an analytical relation for the time-dependent self-energy. The effective self-energy represents the contribution to the moving dot energy, due to interactions between the oscillating dot and the leads it is coupled to. The retarded self-energy of the oscillating dot due to lead  $\alpha$  is given by

$$\Sigma_{n,n'}^r(t, t_1) = \phi_{n,m}(t) g_{\alpha,\alpha}^r(t, t_1) \phi_{n',m}^*(t_1), \quad (\text{A1})$$

where the uncoupled Green's function  $g_{\alpha,\alpha}^r(t, t_1)$  in the leads is

$$\begin{aligned} g_{\alpha,\alpha}^r(t, t_1) &= \frac{1}{N} \sum_j g_{\alpha,j}^r(t, t_1) = \int_{-\infty}^{+\infty} n_\alpha d\varepsilon_\alpha g_\alpha^r(t, t_1) \quad (\text{A2}) \\ &= -i\theta(t - t_1) \int_{-\infty}^{+\infty} d\varepsilon_\alpha n_\alpha \exp[-i(\varepsilon_\alpha + (m + \frac{1}{2})\hbar\omega)(t - t_1)], \end{aligned}$$

and  $\sum_j \Rightarrow \int_{-\infty}^{+\infty} N n_\alpha d\varepsilon_\alpha$ , where  $j$  stands for every channel in each lead,  $n_\alpha$  is the density of states in lead  $\alpha$ ,  $g_{\alpha,j}^r(t, t_1)$  is the uncoupled Green's function for every channel in the leads. The tunneling matrix  $\phi_{n,m}(t)$  is written as

$$\begin{aligned} \phi_{n,m}(t) &= \left\langle V_0(t) e^{\mp \xi \hat{x}} \right\rangle \\ &= \left\{ \int A_n^* e^{-\frac{(x-x_0)^2}{2l^2}} H_n\left(\frac{x-x_0}{l}\right) \right. \\ &\quad \left. V_0(t) e^{\mp \xi \hat{x}} \right. \\ &\quad \left. A_m e^{-\frac{(x')^2}{2l^2}} H_m\left(\frac{x'}{l}\right) \right\} dx, \end{aligned} \quad (\text{A3})$$

where  $x$  is the coordinate of the oscillator,  $\xi$  being the inverse tunneling length.

Using the expressions of the tunneling matrix and the uncoupled retarded Green's function in equation (A1), the retarded self-energy may be written as

$$\begin{aligned} \Sigma_{n,n'}^r(t, t_1) &= \sum_m -i\theta(t-t_1) \int_{-\infty}^{+\infty} N d\varepsilon_\alpha \frac{|V|^2 \theta(t)\theta(t_1)}{N} n_\alpha \exp[-i(\varepsilon_\alpha + (m + \frac{1}{2})\hbar\omega)(t-t_1)] \\ &\quad \times \int dx A_n e^{-\frac{(x-x_0)^2}{2l^2}} H_n\left(\frac{x-x_0}{l}\right) V_0 e^{\mp \xi \hat{x}} A_m^* e^{-\frac{(x')^2}{2l^2}} H_m\left(\frac{x'}{l}\right) \\ &\quad \times \int dx' A_{n'}^* e^{-\frac{(x'-x_0)^2}{2l^2}} H_{n'}\left(\frac{x'-x_0}{l}\right) V_0 e^{\mp \xi \hat{x}'} A_m e^{-\frac{(x')^2}{2l^2}} H_m\left(\frac{x'}{l}\right), \end{aligned} \quad (\text{A4})$$

$$\begin{aligned} &= \sum_m -i\theta(t-t_1) |V|^2 \theta(t)\theta(t_1) n_\alpha \int_{-\infty}^{+\infty} \exp[-i(\varepsilon_\alpha + (m + \frac{1}{2})\hbar\omega)(t-t_1)] d\varepsilon_\alpha \\ &\quad \times \int dx A_n \exp\left(-\frac{(x-x_0)^2}{2l^2}\right) H_n\left(\frac{x-x_0}{l}\right) V_0 e^{\mp \xi \hat{x}} A_m^* \exp\left(-\frac{(x')^2}{2l^2}\right) H_m\left(\frac{x'}{l}\right) \\ &\quad \times \int dx' A_{n'}^* \exp\left(-\frac{(x'-x_0)^2}{2l^2}\right) H_{n'}\left(\frac{x'-x_0}{l}\right) V_0 e^{\mp \xi \hat{x}'} A_m \exp\left(-\frac{(x')^2}{2l^2}\right) H_m\left(\frac{x'}{l}\right), \end{aligned} \quad (\text{A5})$$

$$\begin{aligned} &= -in_\alpha |V|^2 \theta(t)\theta(t_1) \theta(t-t_1) 2\pi \delta(t-t_1) \\ &\quad \times \sum_m \int dx A_n \exp\left(-\frac{(x-x_0)^2}{2l^2}\right) H_n\left(\frac{x-x_0}{l}\right) V_0 e^{\mp \xi \hat{x}} A_m^* \exp\left(-\frac{(x')^2}{2l^2}\right) H_m\left(\frac{x'}{l}\right) \\ &\quad \times \int dx' A_{n'}^* \exp\left(-\frac{(x'-x_0)^2}{2l^2}\right) H_{n'}\left(\frac{x'-x_0}{l}\right) V_0 e^{\mp \xi \hat{x}'} A_m \exp\left(-\frac{(x')^2}{2l^2}\right) H_m\left(\frac{x'}{l}\right), \end{aligned} \quad (\text{A6})$$

where  $\Gamma_\alpha = 4\pi |V|^2 n_\alpha$ . Using the completeness identity,

$$\sum_m A_m^* \exp\left(-\frac{(x)^2}{2l^2}\right) H_m\left(\frac{x}{l}\right) A_m \exp\left(-\frac{(x')^2}{2l^2}\right) H_m\left(\frac{x'}{l}\right) = \delta(x-x')$$

the above equation can be simplified as

$$\begin{aligned} \Sigma_{n,n'}^r(t, t_1) &= -\frac{i\Gamma_\alpha}{2} \theta(t_1) \delta(t-t_1) \\ &\quad \times \int dx' A_n \exp\left(-\frac{(x'-x_0)^2}{l^2}\right) H_n\left(\frac{x'-x_0}{l}\right) V_0 e^{\mp 2\xi \hat{x}'} A_{n'}^* \exp\left(-\frac{(x'-x_0)^2}{2l^2}\right) H_{n'}\left(\frac{x'-x_0}{l}\right), \end{aligned} \quad (\text{A7})$$

After integrating the above expression, we arrive at the

following final result for the retarded self-energy[54],

$$\begin{aligned} \Sigma_{n,n'}^r(t, t_1) &= -\frac{i\Gamma_\alpha}{2} \theta(t_1) \delta(t-t_1) \Sigma^r(\mp), \\ &= \Sigma_\alpha^r(t, t_1) \Sigma^r(\mp) \equiv \Sigma^r(t, t_1) \end{aligned} \quad (\text{A8})$$

with

$$\Sigma^r(\mp) \equiv \psi_{n,n'}^\mp \exp[(\gamma \mp x)^2 - x^2] \quad (\text{A9})$$

where  $\Sigma_\alpha^a(t, t_1) = (\Sigma_\alpha^r(t, t_1))^*$  with  $\alpha$  represents the L or R leads, and the matrices  $\psi_{n,n'}$  is given as

$$\psi_{n,n'}^\mp = \sqrt{\frac{2^{|n'-n|} \min[n, n']!}{\max[n, n']!}} (\mp \gamma)^{|n'-n|} L_{\min[n, n']}^{|n'-n|}(-2\gamma^2), \quad (\text{A10})$$

where the dimensionless tunneling length  $\gamma = \frac{\xi l}{\sqrt{2}}$ ,  $x = \frac{x_0}{l}$ , and the  $-$ ,  $+$  signs stands for the left and the right leads respectively.

Similarly, the lesser self energy may be calculated as

$$\Sigma_{n,n'}^<(t_1, t_2) = \phi_{n,m}(t_1) g_{\alpha,\alpha}^<(t_1, t_2) \phi_{n',m}^*(t_2), \quad (\text{A11})$$

where  $g_{\alpha,\alpha}^<(t_1, t_2)$  is the uncoupled Green's function in the leads and is given as

$$g_{\alpha,\alpha}^<(t_1, t_2) = \frac{1}{N} \sum_j g_{\alpha,j}^<(t_1, t_2) = \int_{-\infty}^{+\infty} n_\alpha d\varepsilon_\alpha g_\alpha^<(t_1, t_2) \quad (\text{A12})$$

$$= \int_{-\infty}^{+\infty} 2in_\alpha f(\varepsilon_\alpha) B_m d\varepsilon_\alpha \exp[-i\varepsilon_\alpha(t_1 - t_2)],$$

We are going to consider that temperature is zero in the leads. So, we assume, when the oscillator appear in the leads it will always be in its ground state such that  $m = 0$  ( $B_m = \delta_{m,0}$ ) and the Fermi distribution function can be replaced with the theta function which in turn limits the integral. With the help of these approximations, and using the expressions for the tunneling matrix and the uncoupled retarded Green's function into equation (A11), the lesser self-energy may be written as

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$$\begin{aligned} \Sigma_{n,n'}^<(t_1, t_2) &= \int_{-\infty}^{\epsilon_{F\alpha} + \frac{1}{2}\hbar\omega} N 2in_\alpha d\varepsilon_\alpha \frac{|V|^2}{N} \theta(t_1) \theta(t_2) \exp[-i\varepsilon_\alpha(t_1 - t_2)] \\ &\times \int dx A_n \exp\left(-\frac{(x-x_0)^2}{2l^2}\right) H_n\left(\frac{x-x_0}{l}\right) V_0 e^{\mp \xi \hat{x}} A_0^* \exp\left(-\frac{(x)^2}{2l^2}\right) \\ &\times \int dx' A_{n'}^* \exp\left(-\frac{(x'-x_0)^2}{2l^2}\right) H_{n'}\left(\frac{x'-x_0}{l}\right) V_0 e^{\mp \xi \hat{x}'} A_0 \exp\left(-\frac{(x')^2}{2l^2}\right), \end{aligned} \quad (\text{A13})$$

$$\begin{aligned} &= 2in_\alpha |V|^2 \theta(t_1) \theta(t_2) \int_{-\infty}^{\epsilon_{F\alpha} + \frac{1}{2}\hbar\omega} d\varepsilon_\alpha \exp[-i\varepsilon_\alpha(t_1 - t_2)] \\ &\times \int dx A_n \exp\left(-\frac{(x-x_0)^2}{2l^2}\right) H_n\left(\frac{x-x_0}{l}\right) V_0 e^{\mp \xi \hat{x}} A_0^* \exp\left(-\frac{(x)^2}{2l^2}\right) \\ &\times \int dx' A_{n'}^* \exp\left(-\frac{(x'-x_0)^2}{2l^2}\right) H_{n'}\left(\frac{x'-x_0}{l}\right) V_0 e^{\mp \xi \hat{x}'} A_0 \exp\left(-\frac{(x')^2}{2l^2}\right), \end{aligned} \quad (\text{A14})$$

$$\begin{aligned} &= i\Gamma_\alpha \theta(t_1) \theta(t_2) \int_{-\infty}^{\epsilon_{F\alpha} + \frac{1}{2}\hbar\omega} \frac{d\varepsilon_\alpha}{2\pi} \exp[-i\varepsilon_\alpha(t_1 - t_2)] \\ &\times \int dx A_n \exp\left(-\frac{(x-x_0)^2}{2l^2}\right) H_n\left(\frac{x-x_0}{l}\right) V_0 e^{\mp \xi \hat{x}} A_0^* \exp\left(-\frac{(x)^2}{2l^2}\right) \\ &\times \int dx' A_{n'}^* \exp\left(-\frac{(x'-x_0)^2}{2l^2}\right) H_{n'}\left(\frac{x'-x_0}{l}\right) V_0 e^{\mp \xi \hat{x}'} A_0 \exp\left(-\frac{(x')^2}{2l^2}\right), \end{aligned} \quad (\text{A15})$$



where  $\Gamma_\alpha = 4\pi |V_{0,\alpha}|^2 n_\alpha$ , with  $\alpha$  representing the L or R leads, and the above equation can be rewritten as

$$\begin{aligned} \Sigma_{n,n'}^<(t_1, t_2) &= i\Gamma_\alpha \theta(t_1) \theta(t_2) \int_{-\infty}^{\epsilon_{F\alpha} + \frac{1}{2}\hbar\omega} \frac{d\varepsilon_\alpha}{2\pi} \exp[-i\varepsilon_\alpha(t_1 - t_2)] \\ &\times \int dx' A_n \exp\left(-\frac{(x' - x_0)^2}{l^2}\right) H_n\left(\frac{x' - x_0}{l}\right) V_0 e^{\mp \xi \hat{x}'} A_0^* \exp\left(-\frac{x'^2}{2l^2}\right) \\ &\times \int dx A_{n'} \exp\left(-\frac{(x - x_0)^2}{2l^2}\right) H_{n'}\left(\frac{x - x_0}{l}\right) V_0 e^{\mp \xi \hat{x}} A_0^* \exp\left(-\frac{x^2}{2l^2}\right), \end{aligned} \quad (A16)$$

Which can be simplified[54] by carrying out the integrals and the final result is written as

$$\begin{aligned} \Sigma_{n,n'}^<(t_1, t_2) &= i\Gamma_\alpha \theta(t_1) \theta(t_2) \frac{\exp[-\frac{x^2}{2} + (\frac{\gamma \mp x}{2})^2]}{\sqrt{n!}} [\mp(\frac{\gamma \pm x}{2})]^n \\ &\times \frac{\exp[-\frac{x^2}{2} + (\frac{\gamma \mp x}{2})^2]}{\sqrt{n'!}} [\mp(\frac{\gamma \pm x}{2})]^{n'} \int_{-\infty}^{\epsilon_{F\alpha} + \frac{1}{2}\hbar\omega} \frac{d\varepsilon_\alpha}{2\pi} \exp[-i\varepsilon_\alpha(t_1 - t_2)], \\ &= \Sigma^<(\mp) \Sigma_\alpha^<(t_1, t_2) \equiv \Sigma^<(t_1, t_2) \end{aligned} \quad (A17)$$

where  $\gamma = \frac{l\xi}{\sqrt{2}}$ ,  $x = \frac{x_0}{l}$ , and the  $-$ ,  $+$  signs stands for the left and the right leads respectively.

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\*Permanent address: Department of Physics, University of Sargodha, Sargodha, Pakistan; m.tahir@uos.edu.pk, m.tahir06@imperial.ac.uk

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